



Aalborg Universitet

AALBORG UNIVERSITY  
DENMARK

## Predicting the Composition Dependence of Glass Hardness

Smedskjær, Morten Mattrup; Mauro, John C.; Yue, Yuanzheng

*Publication date:*  
2011

*Document Version*  
Early version, also known as pre-print

[Link to publication from Aalborg University](#)

*Citation for published version (APA):*

Smedskjær, M. M., Mauro, J. C., & Yue, Y. (2011). *Predicting the Composition Dependence of Glass Hardness*. Abstract from 5th International Workshop on Flow and Fracture of Advanced Glasses, St-Malo, France.

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal -

### Take down policy

If you believe that this document breaches copyright please contact us at [vbn@aub.aau.dk](mailto:vbn@aub.aau.dk) providing details, and we will remove access to the work immediately and investigate your claim.

# Predicting the Composition Dependence of Glass Hardness

Morten M. Smedskjaer,<sup>a,\*</sup> John C. Mauro,<sup>b</sup> and Yuanzheng Yue<sup>a</sup>

<sup>a</sup> *Section of Chemistry, Aalborg University, DK-9000 Aalborg, Denmark*

<sup>b</sup> *Science and Technology Division, Corning Incorporated, Corning, NY 14831, USA*

\* Corresponding author. Tel.: +45 99407240. *E-mail address:* m.smedskjaer@gmail.com

Hardness is an important mechanical property of glasses, but direct calculation of hardness from first principles has shown to be too complex. Temperature-dependent constraint theory has recently been successfully applied to predict the composition dependence of dynamic properties such as glass transition temperature and liquid fragility index. Here, we extend this theory to quantitatively predict hardness of glasses, taking the ternary soda-lime-borate glassy system as an example. By comparison of modeling results with experimental data, we show that hardness is governed by the number of network constraints at room temperature and that a critical number of constraints is required for a material to display mechanical resistance. Furthermore, by applying a surface diffusion process, we have modified the surface composition of the borate glasses. We show that the resulting change in hardness can be predicted by considering the number of room temperature constraints in the modified surface layer. Our result implies that constraint theory may be used as a tool for predicting the composition dependence of other mechanical properties.